Time-convolutionless stochastic Schrödinger equation for open quantum systems

Robert Biele,[1,2,*] Carsten Timm,[1] and Roberto D'Agosta[2,3,†]

[1] *Institute of Theoretical Physics, Technische Universität Dresden, D-01062 Dresden, Germany*
[2] *ETSF Scientific Development Center, Departamento de Física de Materiales, Universidad del País Vasco, E-20018 San Sebastián, Spain*
[3] *IKERBASQUE, Basque Foundation for Science, E-48011, Bilbao, Spain*

(Dated: February 27, 2013)

Stochastic methods form a general framework for investigating the generally non-Markovian dynamics of a quantum-mechanical system coupled to an environment. They promise to be computationally superior to the master-equation approach, which is numerically expensive for large dimensions of the system Hilbert space. A stochastic Schrödinger equation that is local in time but nevertheless reproduces the dynamics of a non-Markovian master equation would be particularly useful. Here, we derive such an equation, which can be solved with moderate numerical cost, comparable to that of a Markovian system. We also discuss a portable algorithm for the generation of the noise associated with the non-Markovian dynamics.

The use of stochastic methods to investigate the dynamics of a physical system coupled to an external bath has a long history dating back to Einstein and Langevin [1, 2]. The idea behind this approach is that the many degrees of freedom of the bath induce random motion in the system [3–7]. Classically, this is due to collisions between the particles of the bath and of the system and can be described by a Langevin equation for certain variables of the system. Quantum-mechanically, the randomness is introduced by transitions between different states of the system induced by the environment and can be described by a stochastic Schrödinger equation (SSE). Alternatively, one can derive statistical descriptions averaging over many realization of the stochastic process, leading to the Fokker-Planck equation for the distribution function of a classical system and the master equation for the reduced density operator of a quantum system [3–7]. Assuming the equivalence between the master equation and the SSE, the latter has sometimes been seen as a "quick and dirty" way to obtain the solution of the former, especially when accurate results were not necessary. Recently, however, it has been shown that the two approaches are not equivalent and the master-equation description might fail when the Hamiltonian is stochastic or depends on the instantaneous state of the system [8]. The numerical solution of the master equation also scales poorly with the number of states kept in the calculation since it is an equation of motion for a *matrix* in state space, whereas a Schrödinger equation is an equation for a *vector*.

The dynamics of an open system is generally non-Markovian. However, the solution of a non-Markovian master equation is difficult because it involves the evaluation of a convolution integral which depends on the history of the system. Therefore, one often employs a Markov approximation, which replaces the memory kernel in this convolution integral by a δ function. We are interested in the thermal relaxation dynamics: In contact with an external bath, the system will approach an equilibrium state. It can be shown that in the non-Markovian case there exists an exact condition that the bath correlation function has to satisfy for the system to reach thermal equilibrium [9]. This condition is no longer satisfied if the Markov approximation is made [9].

In order to study non-Markovian dynamics it would be advantageous to have a SSE that is local in time but is nevertheless able to reproduce the dynamics induced by a non-Markovian master equation. In this Letter, we introduce a local-in-time (time-convolutionless) SSE and show its equivalence to a non-Markovian master equation. Finally, we illustrate this SSE by studying the thermal relaxation of an electronic system coupled to the electromagnetic field in a cavity.

Our starting point is a standard second-order master equation [3, 5]. This non-Markovian master equation (NMME) is quite generic, no restrictions on the form of the coupling between the system and the environment are imposed, except that this coupling is bilinear, $\hat{H}_{\rm int} = \lambda \sum_a \hat{S}_a \otimes \hat{B}_a$, in the operators $\hat{S}_a$ and $\hat{B}_a$ from the system and the bath, respectively. Here we assume that $\hat{S}_\alpha$ and $\hat{B}_\alpha$ are hermitian operators, the extension to the more general case where only $\hat{H}_{\rm int}$ is hermitian is straightforward. Under the assumptions of weak system-bath interaction and factorization of the full density operator at the initial time $t = 0$, the equation of motion for the reduced density operator $\hat{\rho}$ of the system is given by (setting $\hbar = 1$)

$$\frac{d\hat{\rho}(t)}{dt} = -i\big[\hat{H}, \hat{\rho}(t)\big] + \lambda^2 \sum_a [\hat{S}_a, \hat{M}_a^\dagger(t) - \hat{M}_a(t)] \quad (1)$$

with

$$\hat{M}_a(t) \equiv \sum_b \int_0^t d\tau\, c_{ab}(t,\tau) e^{-i\hat{H}(t-\tau)} \hat{S}_b \hat{\rho}(\tau) e^{i\hat{H}(t-\tau)}. \quad (2)$$

In this NMME, $\hat{H}$ is the Hamiltonian of the system and the correlation kernel is given by $c_{ab}(t,\tau) \equiv$

$\mathrm{Tr}_B[\hat{\rho}_B^{\mathrm{eq}}\hat{B}_a(t)\hat{B}_b(\tau)]$, where the trace is over the environmental degrees of freedom, $\hat{B}_a(t) \equiv e^{i\hat{H}_B t}\hat{B}\, e^{-i\hat{H}_B t}$, and $\hat{H}_B$ is the Hamiltonian of the environment. Here, $\hat{\rho}_B^{\mathrm{eq}}$ is the statistical operator of the bath at time 0, which we assume to be the one for thermal equilibrium. Hence, $\hat{\rho}_B^{\mathrm{eq}}$ introduces the temperature into the description of the dynamics. This should imply that the system in contact with the bath is driven toward a steady state that coincides with the thermal equilibrium of the system, $\hat{\rho}(t\to\infty) \propto \exp(-\beta\hat{H})$, with the same temperature as the bath [10]. This is the case if the power spectrum $C_{ab}(\omega) \equiv \int_{-\infty}^{\infty} dt\, c_{ab}(t)\, e^{-i\omega t}$ satisfies the detailed-balance condition [9]

$$C_{ab}(-\omega) = e^{\beta\omega} C_{ba}(\omega). \tag{3}$$

Gaspard and Nagaoka [11] have shown that the dynamics introduced by the NMME can be obtained not only by a numerical integration of Eq. (1) but also by the solution of a SSE for a state $|\Psi(t)\rangle$,

$$\begin{aligned} i\partial_t|\Psi(t)\rangle &= \hat{H}|\Psi(t)\rangle + \lambda\sum_a \gamma_a(t)\hat{S}_a|\Psi(t)\rangle \\ &\quad - i\lambda^2\sum_{a,b}\hat{S}_a\int_0^t dt' c_{ab}(t')e^{-i\hat{H}t'}\hat{S}_b|\Psi(t-t')\rangle. \end{aligned} \tag{4}$$

In this non-Markovian SSE (NMSSE) the complex noises $\gamma_a(t)$ have the properties

$$\overline{\gamma_a(t)} = 0, \quad \overline{\gamma_a(t)\gamma_b(t')} = 0, \quad \overline{\gamma_a^*(t)\gamma_b(t')} = c_{ab}(t-t') \tag{5}$$

and one can obtain the dynamics of the open quantum system by an average over realizations of the stochastic process, indicated by the overline. In particular, the reduced density operator is obtained as $\hat{\rho}(t) = \overline{|\Psi(t)\rangle\langle\Psi(t)|}$. However, any attempt to solve the NMSSE (4) requires a large numerical effort due to the time integral, which needs to be evaluated at every time step and for every realization. This begs the question of whether one can find a simpler SSE that reproduces on average the dynamics induced by the NMME. In the following we present such a SSE.

We will show that the time-convolutionless SSE (TCLSSE)

$$i\partial_t|\Psi(t)\rangle = \left(\hat{H} + \lambda\sum_a \gamma_a(t)\hat{S}_a - i\lambda^2\hat{T}(t)\right)|\Psi(t)\rangle \tag{6}$$

with

$$\hat{T}(t) \equiv \sum_{a,b}\hat{S}_a\int_0^t dt'\, c_{ab}(t')\, e^{-i\hat{H}t'}\hat{S}_b e^{i\hat{H}t'} \tag{7}$$

reproduces on average the dynamics induced by the NMME (1) up to fourth order in λ. To prove this, we write Eq. (6) in the interaction picture, $|\Psi_I(t)\rangle = e^{i\hat{H}t}|\Psi(t)\rangle$ and $\hat{S}_a(t) = e^{i\hat{H}t}\hat{S}_a e^{-i\hat{H}t}$, and expand the time-evolution operator up to second order in λ,

$$\begin{aligned} |\Psi_I(t)\rangle \cong \Bigg[\mathbb{1} &- i\lambda\sum_a\int_0^t dt_1\,\gamma_a(t_1)\hat{S}_a(t_1) \\ &- \lambda^2\sum_{a,b}\int_0^t dt_1\int_0^{t_1} dt_2\, c_{ab}(t_2)\hat{S}_a(t_1)\hat{S}_\beta(t_1-t_2) \\ &- \lambda^2\sum_{a,b}\int_0^t dt_1\int_0^{t_1} dt_2\,\gamma_a(t_1)\hat{S}_a(t_1)\gamma_b(t_2)\hat{S}_b(t_2)\Bigg] \\ &\times|\Psi_I(0)\rangle + \mathcal{O}(\lambda^3). \end{aligned} \tag{8}$$

This expansion is inserted into the expression for the reduced density operator $\hat{\rho}_I(t) = \overline{|\Psi_I(t)\rangle\langle\Psi_I(t)|}$. By performing the average, using the properties in Eq. (5) and the identity $c_{ab}(\tau,t) = c_{ba}^*(t,\tau)$, and differentiating with respect to t we arrive at

$$\begin{aligned} \partial_t\hat{\rho}_I(t) \;=\; \lambda^2\sum_{a,b}\int_0^t d\tau\,\big[&c_{ab}(t,\tau)\hat{S}_b(\tau)\hat{\rho}_I(0)\hat{S}_a(t) \\ &- c_{ab}(t,\tau)\hat{S}_a(t)\hat{S}_b(\tau)\hat{\rho}_I(0) \\ &+ c_{ab}^*(t,\tau)\hat{S}_a(t)\hat{\rho}_I(0)\hat{S}_b(\tau) \\ &- c_{ab}^*(t,\tau)\hat{\rho}_I(0)\hat{S}_b(\tau)\hat{S}_a(t)\big] + \mathcal{O}(\lambda^4). \end{aligned} \tag{9}$$

Note that the averages of the terms in λ^3 vanish. Furthermore, replacing $\rho_I(0)$ by $\rho_I(\tau) + \mathcal{O}(\lambda^2)$ does not change the equation up to terms in λ^4. Finally, by returning to the Schrödinger picture we arrive at the NMME (1) up to terms of order λ^4, i.e., higher than the order up to which these equations are valid. This is remarkable since one might expect a more complex time-non-local SSE to be required for reproducing the dynamics of the NMME (1). Still, the TCLSSE is local in time, i.e., the operator $\hat{T}(t)$ does not depend on the state of the system at previous times and thus can be calculated before the numerical integration and be used for each realization of the stochastic process. Hence, the numerical cost of solving each realization of the TCLSSE is comparable to that of a Markovian SSE [4, 11]. However, the proposed TCLSSE requires the generation of colored noise and thus the method will only be practicable if an efficient algorithm for the generation of this noise is available.

Such an algorithm indeed exists, as we show below. We consider only a single bath operator; the generalization to several bath operators is straightforward. Existing algorithms for the generation of (real) colored noise rely on the numerical solution of a stochastic differential equation that has to produce noise with the given target correlation function $c(t)$ [12]. However, such an equation is a piece of information that is rarely available, since even the analytic expression of $c(t)$ may not be known. Except for a few simple models, it is more common to have access to the power spectrum $C(\omega)$. Indeed, $C(\omega)$ is connected with the transitions in the bath. The algorithm presented in Ref. [13] does not only require $C(\omega)$

but also the inverse Fourier transform of its square root. This quantity is then convoluted with a white noise to generate the target real colored noise. We will introduce an algorithm that directly uses $\sqrt{C(\omega)}$ as input, thereby reducing the numerical cost compared to the algorithm of Ref. [13] and that generates a complex colored noise.

In the following, we present a portable algorithm to generate complex colored noise with the properties in Eq. (5), taking a given power spectrum $C(\omega)$ as input. One can easily prove that the noise $\gamma(t)$ can be generated by the relation

$$\gamma(t) = \int_{-\infty}^{\infty} \frac{d\omega}{\sqrt{2\pi}} \sqrt{C(\omega)}\, x(\omega)\, e^{i\omega t}, \qquad (10)$$

where $x(\omega)$ is a white-noise process in the frequency domain satisfying

$$\overline{x(\omega)} = 0,\ \overline{x(\omega)x(\omega')} = 0,\ \overline{x^*(\omega)x(\omega')} = \delta(\omega - \omega'). \quad (11)$$

By substituting the definition (10) into $\overline{\gamma^*(t)\gamma(t')}$ and using Eq. (11), we immediately arrive at Eq. (5). The other relations in Eq. (5) are proven in a similar way. From a numerical point of view, the generation of this colored noise requires the calculation of the Fourier transform in Eq. (10). A similar algorithm restricted to real noise has been proposed in the past [14, 15].

In order to compare our algorithm with the two from Refs. [13] and [14, 15], we choose a test function for which we know $c(t)$ and $C(\omega)$ analytically, namely $c(t) = e^{-t^2/2\sigma^2}/(2\pi\sigma^2)^{1/4}$ and $C(\omega) = (2\pi\sigma^2)^{1/4}\, e^{-\omega^2\sigma^2/2}$. We fix $\sigma = 1$ as our unit of time and choose the interval $t \in [-25, 25]$ for the numerical Fourier transformation. To quantify the agreement between the target $c(t)$ and the approximations given by the three algorithms we use the relative error $\delta_c = \int_{-\infty}^{\infty} dt\, |c(t) - \overline{\gamma(0)\gamma^*(t)}|^2 / \int_{-\infty}^{\infty} dt\, |c(t)|^2$.

In Fig. 1 we report the computational cost of calculating the correlation function $c(t)$ vs. the number of discretization steps of the time interval, N. Our algorithm is moderately faster than the others for any value of N. In the inset of Fig. 1, we show the relative error δ_c calculated for 1024 time steps by averaging over an increasing number of realizations of the noise. The new method gives the best approximation, i.e., the minimum δ_c, for any number of runs. While this computational gain is of little importance, the main advantages of the new method are that it works directly with the given power spectrum and produces a complex noise.

Finally, we illustrate our results by discussing how the TCLSSE is able to reproduce the dynamics induced by the NMME and how it describes thermal relaxation for a specific system. We consider the coupling of an electronic system to the electromagnetic field in a three-dimensional cavity. In the dipole approximation, one can derive from first principles the power spectrum for this system (we

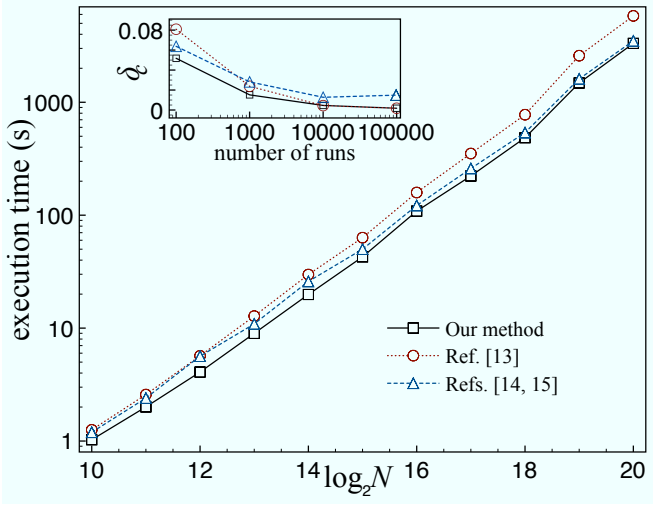

FIG. 1: (Color online) Computation time as a function of the number of time steps N for our method compared to those of Refs. [13] and [14, 15]. Inset: Relative error for $N = 1024$ time steps calculated by averaging over an increasing number of realizations of the noise.

set the speed of light to unity)

$$C_{\mathrm{cav}(\omega)} = \frac{|\omega|^3}{\pi V \epsilon_0} \left[n_B(|\omega|) + \theta(-\omega)\right] \quad \text{for} \quad |\omega| < \omega_c, \qquad (12)$$

where $n_B(\omega) \equiv 1/(e^{\beta\omega} - 1)$ is the Bose-Einstein distribution function, $\theta(\omega)$ is the Heaviside step function, V is the volume of the cavity, and ω_c is a cutoff frequency determined by the dimensions of the system. This cutoff is necessitated by the assumption made in the dipole approximation that the electromagnetic field is uniform in the region of space of the system. For $|\omega| > \omega_c$, the power spectrum is set to vanish [16]. One can show that the detailed-balance condition (3) is satisfied by this power spectrum. Since for this model system the correlation function $c(t)$ is not given in an analytical form, we will use Eq. (10) to generate the noise.

In order to quantify the agreement between the noise generated by Eq. (10) and the power spectrum in Eq. (12), we have performed a Fourier transform of the time-domain signal and compared it with our target. Figure 2 shows that the agreement is excellent.

For the electronic system we use a three-site tight-binding chain described by the Hamiltonian

$$\hat{H} = -T\left(\hat{c}_1^\dagger \hat{c}_2 + \hat{c}_2^\dagger \hat{c}_1 + \hat{c}_2^\dagger \hat{c}_3 + \hat{c}_3^\dagger \hat{c}_2\right), \qquad (13)$$

where the operators $\hat{c}_i^\dagger$ create an electron at site i, and assume a single electron to be present. This system is coupled to the electromagnetic field inside the cavity by the operator

$$\hat{S} = -q \sum_{l,p} \mathbf{u} \cdot \langle W_l | \mathbf{r} | W_p \rangle\, \hat{c}_l^\dagger \hat{c}_p, \qquad (14)$$

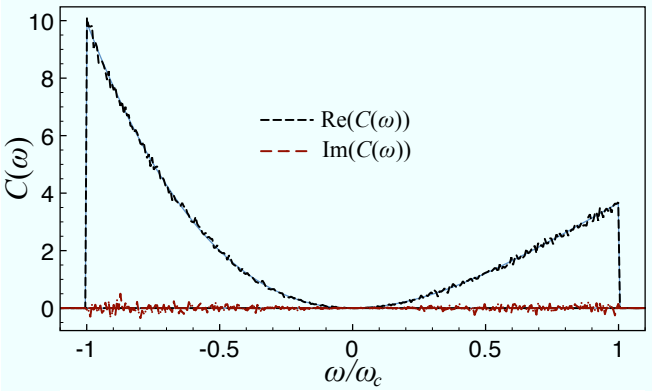

FIG. 2: (Color online) Comparison between the target, Eq. (12) (solid lines) and the Fourier transform into the frequency domain of the correlation function obtained from Eq. (10) by averaging over 90000 realizations of the noise (dashed lines).

where q is the charge of the electron and $|W_i\rangle$ is the state localized at site i. For simplicity, we have assumed that each mode of the cavity has the same polarization direction $\mathbf{u}$, parallel to the tight-binding chain. Note that the form of this operator should be immaterial for the establishment of thermal equilibrium, which is only determined by the power spectrum. Indeed, we can check if the detailed-balance condition is necessary for the system to reach thermal equilibrium. To that end, we use the operator in Eq. (14) within a Markov approximation for the correlation function, $c(t) \propto \delta(t)$. We find that a steady state is approached that does not correspond to thermal equilibrium [9].

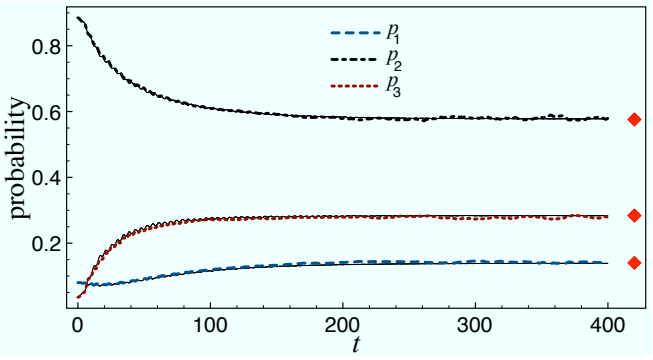

FIG. 3: (Color online) Dynamics of the occupation probabilities of the eigenstates of the Hamiltonian (13) as calculated from the evolution of the TCLSSE (dashed lines) and the NMME (solid lines) with the power spectrum given by Eq. (12). The red diamonds represent the thermal-equilibrium probabilities calculated from Eq. (15).

In Fig. 3 we show the probability of occupying the three eigenstates of the Hamiltonian as a function of time calculated using the TCLSSE (dashed lines) and the NMME (solid lines), respectively. For the TCLSSE the results have been obtained by averaging over 90000 independent realizations of the noise. We have used the parameters $\beta = 1$, $\omega_c = 1$, $T = 1$, and $\lambda = 0.1$ and we have used the Euler algorithm [17, 18] with time step $\Delta t = 0.005$ to numerically solve the equations. The dynamics induced by the NMME and the TCLSSE are in good agreement: The small discrepancies in the numerical solutions are due to the finite number of realizations we have used; the solution of the TCLSSE still contains some noise, as expected. For long times, both formalisms converge to the thermal-equilibrium probabilities

$$p_i = \frac{e^{-\beta\epsilon_i}}{e^{-\beta\epsilon_1} + e^{-\beta\epsilon_2} + e^{-\beta\epsilon_3}}, \tag{15}$$

where ϵ_i are the eigenvalues of the Hamiltonian (13). If we were only interested in the long-time limit, we could have averaged over all times after some equilibration time $t_{\min}$ to obtain better statistics, using the ergodic theorem to replace the average over many realizations with an average over the time evolution of a single realization.

In conclusion, we have introduced a time-local (time-convolutionless) version of a *non-Markovian* stochastic Schrödinger equation, which correctly describes the approach to thermal equilibrium as obtained from a non-Markovian master equation. This equation can be integrated with moderate numerical cost, comparable to that of a Markovian system. It also shows more advantageous scaling with the number of states compared to the master equation, which is particularly useful for larger systems.

R. B. and R. D'A. acknowledge support from MICINN (FIS2010-21282-C02-01 and PIB2010US-00652), the Grupos Consolidados UPV/EHU del Gobierno Vasco (IT-319-07) and ACI-Promociona (ACI2009-1036). R. B. acknowledges financial support from IKERBASQUE, Basque Foundation for Science. C. T. acknowledges financial support by the Deutsche Forschungsgemeinschaft, in part through Research Unit 1154. R. D'A. acknowledges the financial support of the CONSOLIDER-INGENIO 2010 "NanoTherm" (CSD2010-00044) and is thankful for its hospitality to the Physics Department of the King's College London.

* Electronic address: robert.biele@gmx.net
† Electronic address: roberto.dagosta@ehu.es

[1] A. Einstein, Ann. Phys. (Leipzig) **322**, 549 (1905).
[2] P. Langevin, C. R. Acad. Sci. **146**, 530 (1908).
[3] C. W. Gardiner and P. Zoller, *Quantum Noise*, 2nd edition (Springer, Berlin, 2000).
[4] N. G. van Kampen, *Stochastic Processes in Physics and Chemistry*, 3rd edition (Elsevier, Amsterdam, 2007).
[5] U. Weiss, *Quantum Dissipative Systems*, 3rd edition (World Scientific, Singapore, 2007).
[6] P. E. Kloeden and E. Platen, *Numerical Solution of Stochastic Differential Equations*, Applications of Mathematics Series vol. 23 (Springer, Heidelberg, 1999).

[7] M. Razavy, *Classical and Quantum Dissipative Systems* (Imperial College Press, London, 2006).
[8] R. D'Agosta and M. Di Ventra, Phys. Rev. B **78**, 165105 (2008).
[9] R. Biele and R. D'Agosta, arXiv:1112.2694.
[10] It is well-known that the Hamiltonian $\hat{H}$ appearing in this expression might be different from the one describing the system dynamics, due for example to the Lamb shift. For simplicity, we assume these effects can be neglected. Their inclusion would be straightforward.
[11] P. Gaspard and M. Nagaoka, J. Chem. Phys. **111**, 5676 (1999).
[12] R. Mannella and V. Palleschi, Phys. Rev. A **46**, 8028 (1992).
[13] J.-L. Barrat and D. Rodney, J. Stat. Phys. **144**, 679 (2011).
[14] S. O. Rice, Bell Systems Tech. J. **23**, 282 (1944).
[15] K. Y. R. Billah and M. Shinozuka, Phys. Rev. A **42**, 7492 (1990).
[16] Note that increasing ω_c does not change the relaxation dynamics as long as ω_c is larger than the energy differences in the system and hence permits the possible energy transitions.
[17] W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, *Numerical Recipes in Fortran 77: The Art of Scientific Computing* (Cambridge University Press, Cambridge, 2001).
[18] P. E. Kloeden, E. Platen, and H. Schurz, *Numerical Solution of SDE through Computer Experiments*, 3rd edition (Springer, Berlin, 1997).